

METHODS OF DETERMINING LIGAND RESIDUE BINDING AFFINITY

ABSTRACT OF THE DISCLOSURE

Methods and systems for determining the affinity between polypeptide amino acid residues and one or more molecular fragments, and for using the affinity values to aid in drug design including a computer simulation which calculates the interaction energy between a polypeptide and at least one molecular fragment. An affinity value is then assigned to at least one fragment and residue pair if the fragment is in the vicinity of the residue. Affinity values are used to rank fragments, build ligands and determine binding sites.